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Molecular Hospitality: An Examination of the Interactions between Brooker's Merocyanine and Modified Cyclodextrins

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The equilibrium of a guest molecule binding to a host occurs through weak molecular interactions instead of through the formation of chemical bonds. A cyclodextrin (CD) is used as the host molecule due to its basket-like shape which is beneficial to complex formation with the guest molecule, Brooker's merocyanine (BM), which fits well within beta-CD. BM is a highly conjugated dye that can exhibit a charge, allowing for a variety of the weak molecular interactions involved with complex formation, such as hydrogen bonds, to be studied. This project focuses on the effect of different modifications to the CD on the binding constant of BM with a CD host. The binding constant can be determined using the Benesi-Hildebrand equation to process data collected using UV-Vis and fluorescence spectroscopy. The determination of binding constants for multiple different CD modifications, including beta-CD, hydroxypropyl-beta-CD, and triacetyl-beta-CD, will allow for a comparison of how these modifications affect the degree of binding as well as whether or not hydrogen bonding is an important factor in the binding of this host-guest system. A better understanding of the factors that affect binding in host-guest systems will allow for better predictions of their behavior under different conditions.

Information about the Author:
Ben is a junior chemistry major with an interest in food chemistry. He has worked on this project since September 2012 and plans to continue working on cyclodextrin research through his graduation in 2014, with the hopes of working on the isomerization characteristics of the guest within the host. This topic allows him to focus on analytical chemistry, the area he plans to focus on in graduate school. Apart from research and classes, Ben is also involved in VU Science Olympiad, Chemistry Club, Luce Band, and Gamma Theta Upsilon.

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